

EXPERIMENTAL VALIDATION AND COMBUSTION MODELING OF A JP-8 SURROGATE IN A SINGLE CYLINDER DIESEL ENGINE

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Outline

- Objectives
- Properties of Surrogate Vs. its Target JP-8
- Experimental Setup and Test Conditions
- Mechanism Reduction and Validation, CFD Setup
- Results
- Summary and Conclusions

- **Objectives**
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Research Objectives

- Validate a two-component JP-8 surrogate in a single cylinder diesel engine. Validation parameters include
 - Ignition delay
 - Combustion gas pressure, rate of heat release, and mass-averaged cylinder gas temperature
 - Engine-out emissions
- Develop a reduced kinetic model of the two-component surrogate
 - Mechanism reduction and validation
- Conduct 3D CFD simulation, and compare the results of simulation with those of the experimental data for the surrogate. The parameters under comparisons include
 - Ignition delay
 - Combustion gas pressure, rate of heat release, and mass-averaged cylinder gas temperature
 - Engine-out emissions

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Properties of Surrogate Vs. Target JP-8

- The surrogate, named S2, is one of the six surrogates developed and validated in the Ignition Quality Tester.
 - SAE Int. J. Fuels Lubr. 2014-01-9077

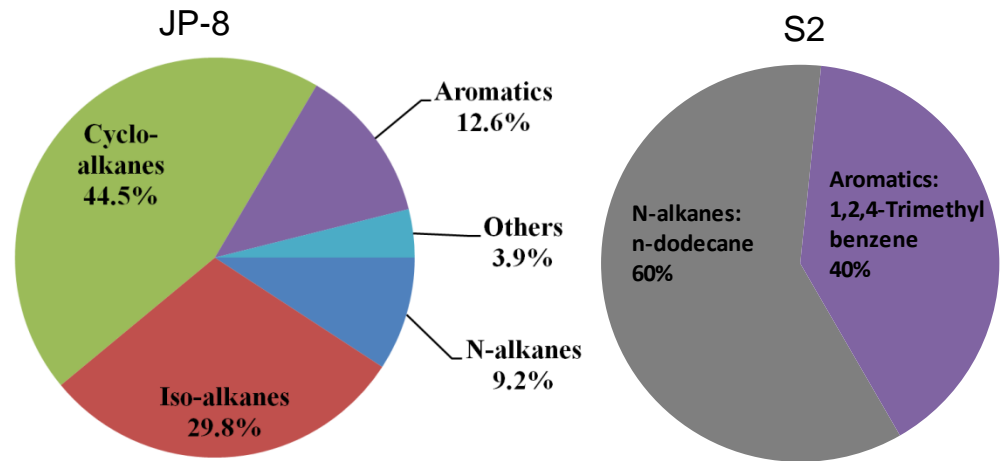


Figure 1. Chemical class composition (%Volume)

Table 1. Properties of JP-8 Vs. Surrogate

Fuels/Properties	JP-8	Surrogate S2
Derived Cetane Number (DCN)	50.1	50.4
Density @ 25°C (g/cc)	0.797	0.802
Lower Heating Value (MJ/kg)	43.3	43.16*
Hydrogen to Carbon (H/C) Ratio	1.93	1.79
Molecular Weight (MW) (g/mole)	160.96	144.06
Threshold Sooting Index (TSI)	22.96	35.27*

* Calculated

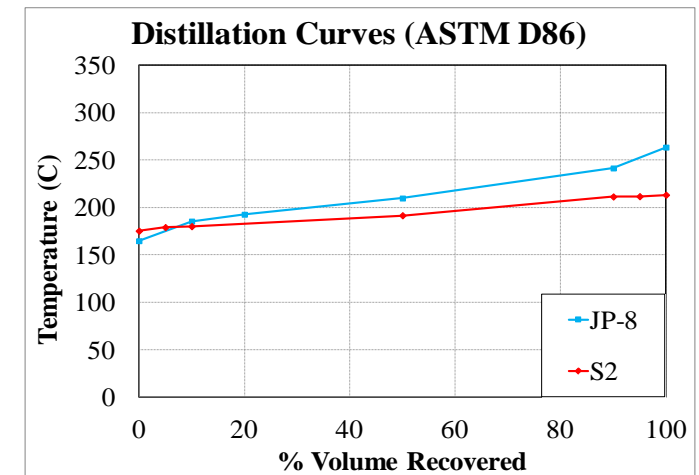


Figure 2. Distillation curves of JP-8 Vs. Surrogate

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Experimental Setup and Test Conditions

ENGINE: PNGV (Partnership for a New Generation of Vehicles)

- Research type, direct injection, four-stroke diesel engine with double overhead camshaft and four valves
 - Horiba Mexa DEGR 7100
 - For recording NO_x, CO, and total hydrocarbons
 - SMPS (Scanning Mobility Particle Sizer)
 - For recording particulate matter concentration

Table 2. Engine Specifications

Engine	Single Cylinder, Four-stroke
Displacement Volume (c.c)	422
Bore (mm) x Stroke (mm)	79.5 x 85
Combustion Chamber	Re-entrant bowl piston
Compression Ratio	20:1
Injection System	Common Rail
Injector Specifications	Solenoid, 6 holes, 320 Minisac, 0.131 mm hole diameter

Table 3. Test Conditions

Engine Load	3 bar IMEP
Engine Speed	1500 RPM
Swirl	3.77
EGR	0 %
Intake Air Temperature	30°C
Intake Air Pressure	1.2 bar
Rail Pressure	800 bar
Start of Injection (CAD)	2.2 bTDC, 0.3 bTDC, 1.8 aTDC

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Mechanism Reduction

- Mechanism Source – CRECK Modeling
 - Version 1212, December 2012
 - 466 species and 14631 reactions, including NOx mechanisms
- Mechanism Reduction
 - Software: Chemical Workbench, Kintech Laboratory, Moscow, Russia
 - Reduction Methods
 - Path Flux Analysis
 - Computational Singular Perturbation
 - Reduction Criterion: Ignition delay error within $\pm 10\%$
 - Reduction Parameters
 - Initial set of target species – Fuel species (n-dodecane and 1,2,4-trimethylbenzene), Air (O_2 and N_2), HO_2 , O, H, OH, H_2O , CO_2 , CO, NO, NO_2 , and inert species (He and Ar)
 - Reduction conditions – Equivalence ratio = 0.5, Temperature = 500-800K
 - Final reduced mechanism
 - 120 species and 1471 reactions

Mechanism Validation

- DARS Basic
 - 0-D
 - Constant volume homogeneous reactor
 - 0 to 10 ms simulation
 - 50-50 mole fractions of n-dodecane and 1,2,4-trimethylbenzene

Table 4. Validation Conditions

Test Variables	Variables Range
Temperature (K)	700 - 1300 ($\Delta T = 50$)
Pressure (bar)	40, 60, 80
Equivalence ratio (Φ)	0.5, 1.0, 2.0

3D CFD Simulation Models, Settings, and Assumptions

- 3D CFD Software – FORTE, Reaction Design, San Diego, USA
- CFD Modules
 - Dynamic cell clustering (DCC)
 - Temperature dispersion = 5 K; Equivalence ratio dispersion = 0.05
- CFD Models
 - Nozzle-flow model – Spray initialization
 - Kelvin-Helmholtz/Rayleigh-Taylor (KHRT) model: Spray atomization and droplet breakup
 - Rosin-Rammler model: Size distribution of child drops
 - Radius of influence model: Droplets collision
 - FORTE's wall impingement model: Droplet-wall interaction
 - O'Rourke and Amsden wall film model: Wall film dynamics (Spray impingement, wall conditions, and near-wall gas flows)
 - Re-Normalized Group Theory (RNG) modified model: In-cylinder turbulent flows
 - FORTE's generalized model: Turbulence-chemistry interaction

- Settings
 - One-sixth sector mesh
 - Sector mesh: 17809 cells at BDC
 - Simulation conducted from IVC (140 CAD bTDC) to EVO (155 CAD aTDC)
- Two assumptions
 - Sinusoidal rate shape was assumed to represent the experimental rate shape
 - FORTE's default values of the model constants were used, and were kept the same for all the simulation cases

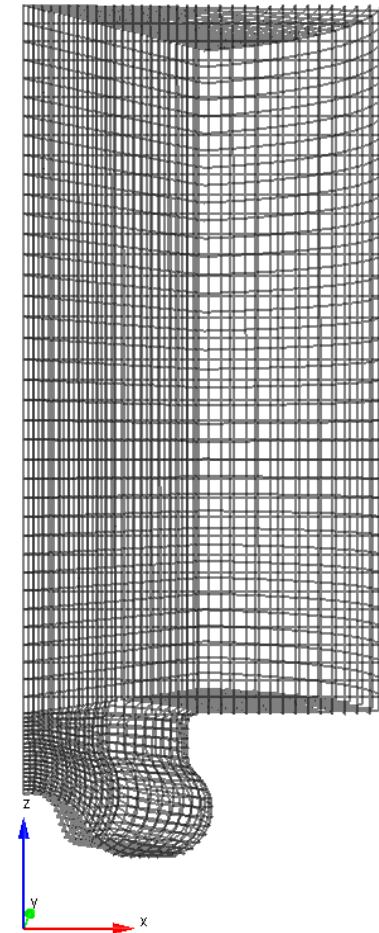


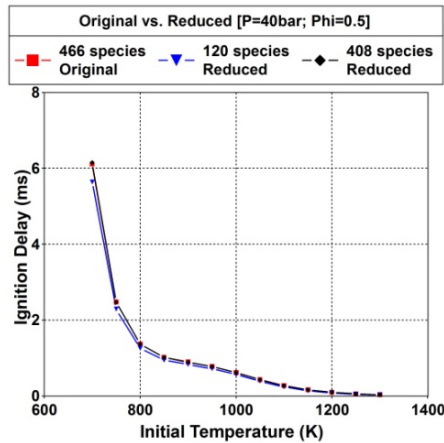
Figure 3. Sector mesh

Outline

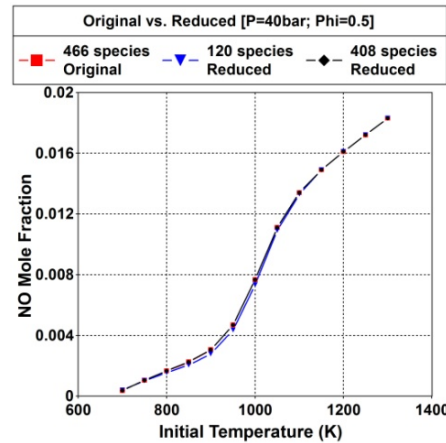
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Results: Mechanism Validation

Ignition Delay



Nitric oxide (NO)



Nitrogen dioxide (NO₂)

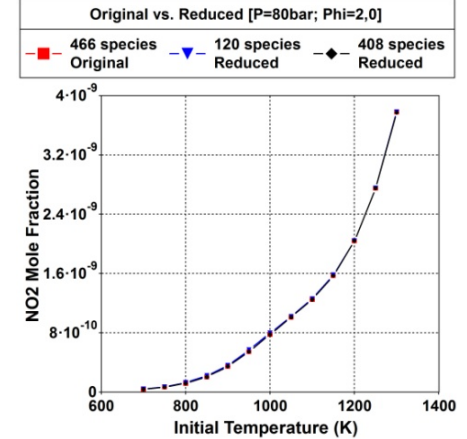
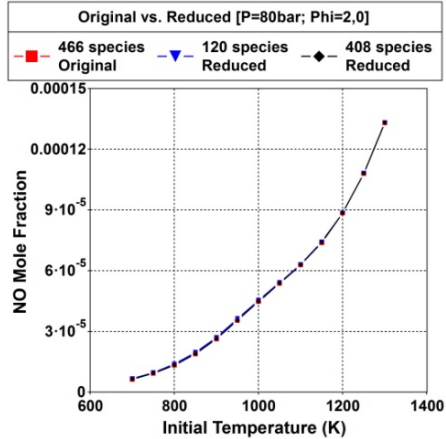
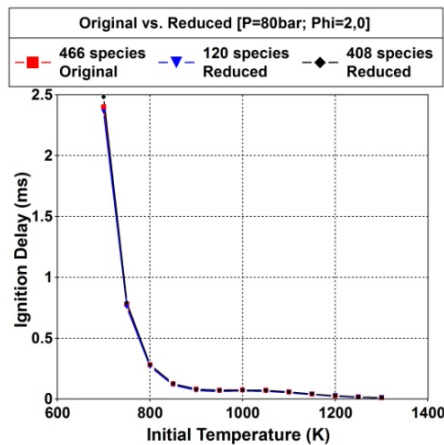
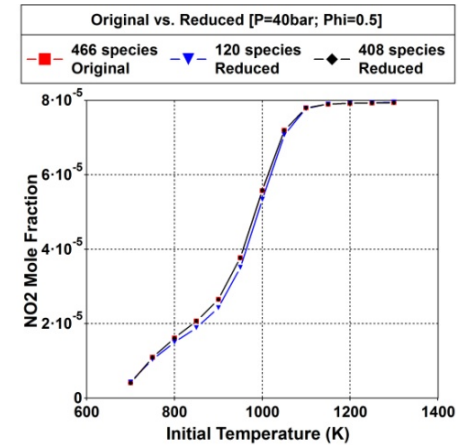


Figure 4. Comparison of reduced and original mechanisms

Results: Experiments/3D CFD Simulation

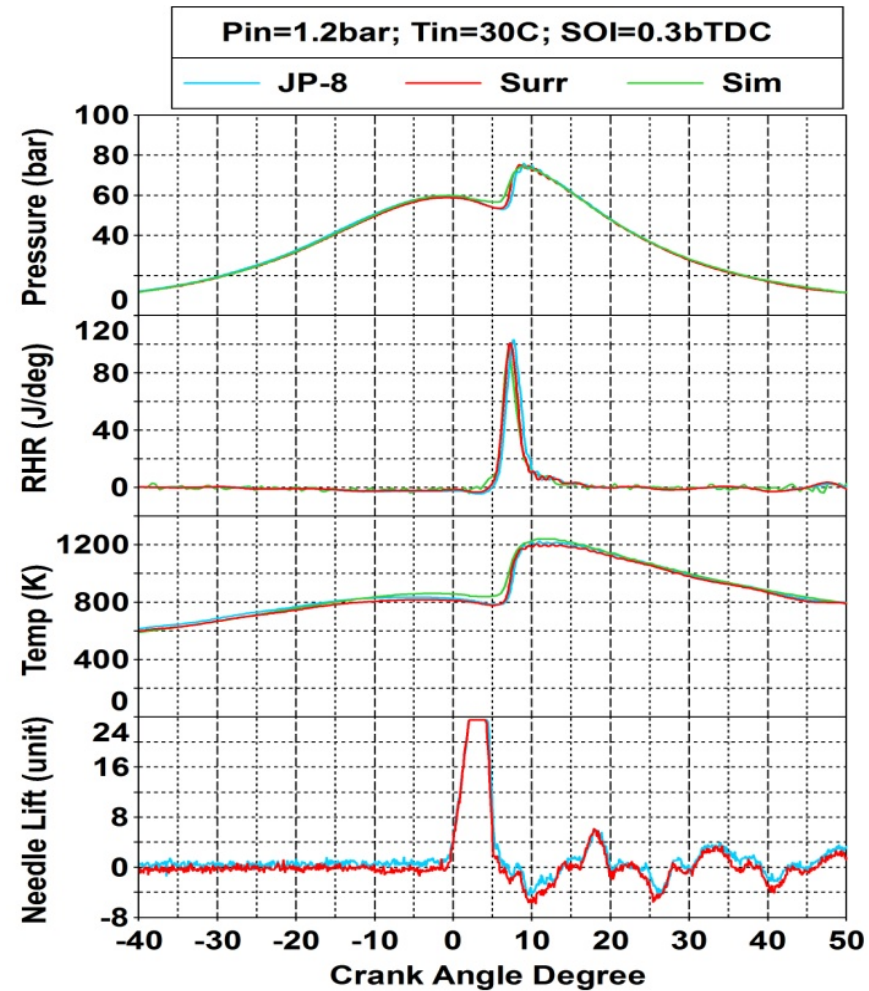
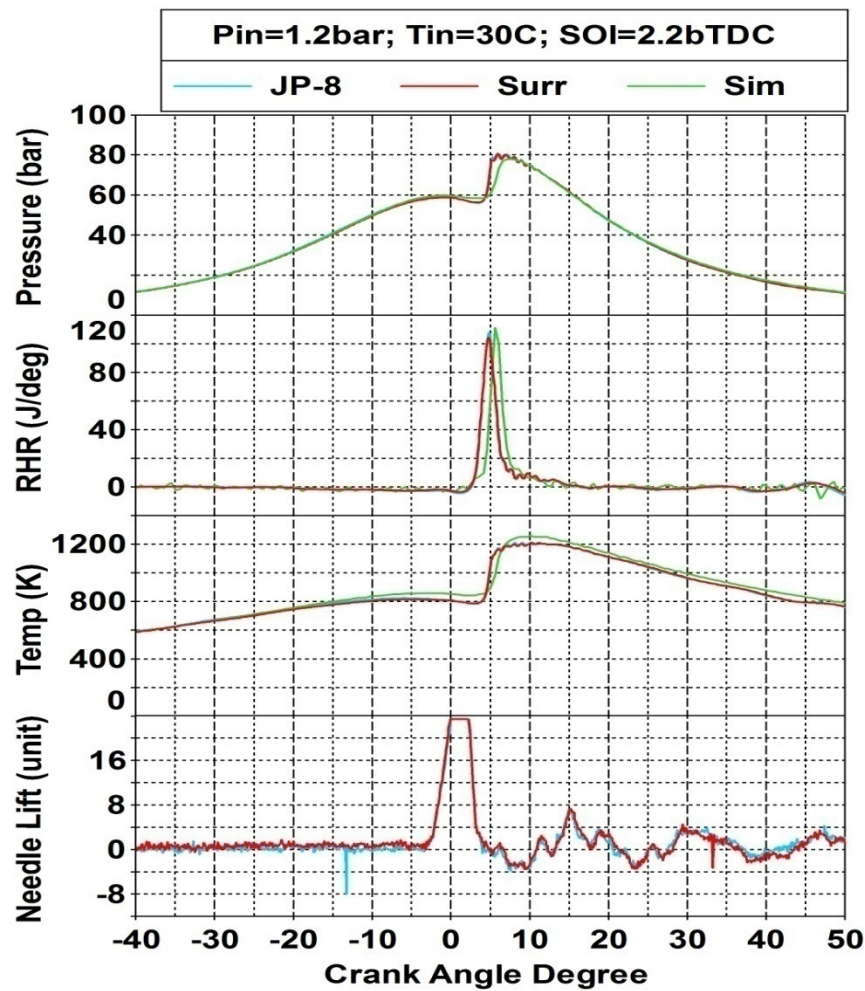


Figure 5. Comparison of cylinder pressure, rate of heat release, mass-averaged gas temperature, and needle lift

Results: Experiments/3D CFD Simulation

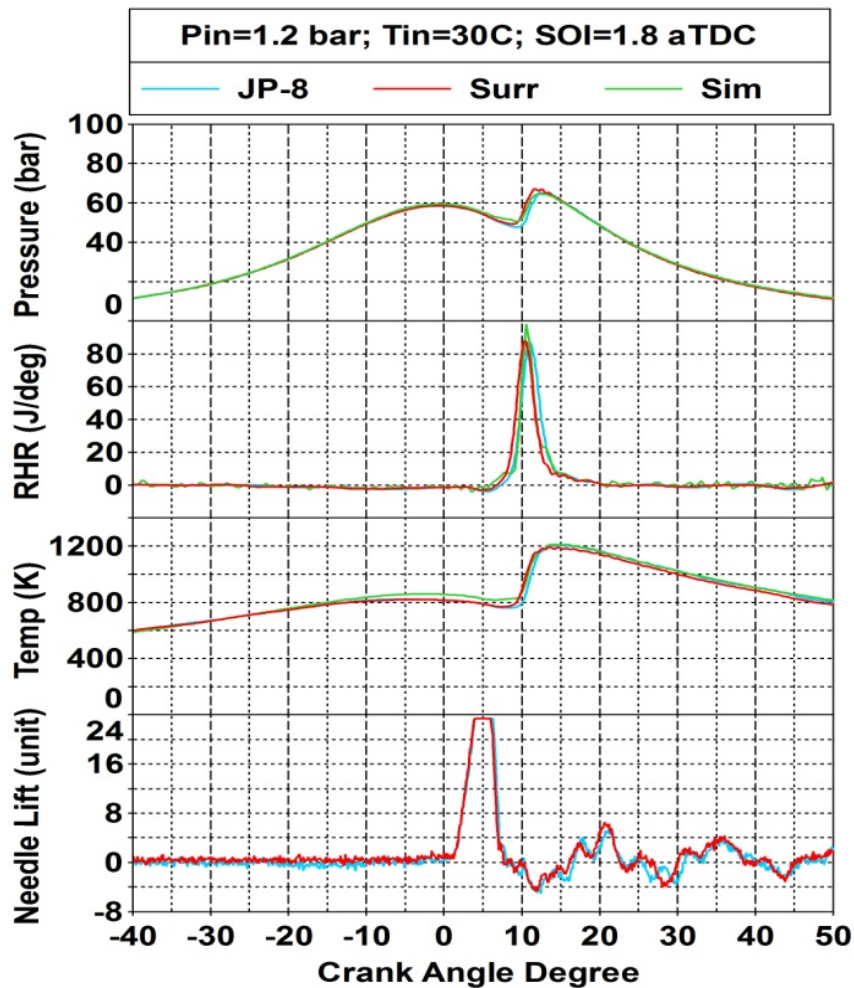


Figure 5. Comparison of cylinder pressure, rate of heat release, mass-averaged gas temperature, and needle lift

Table 5. Experimental fuel rate (gm/min)

Start of Injection (CAD)	JP-8	S2
2.2 bTDC	5.69	5.67
0.3 bTDC	5.68	5.75
1.8 aTDC	5.77	5.65

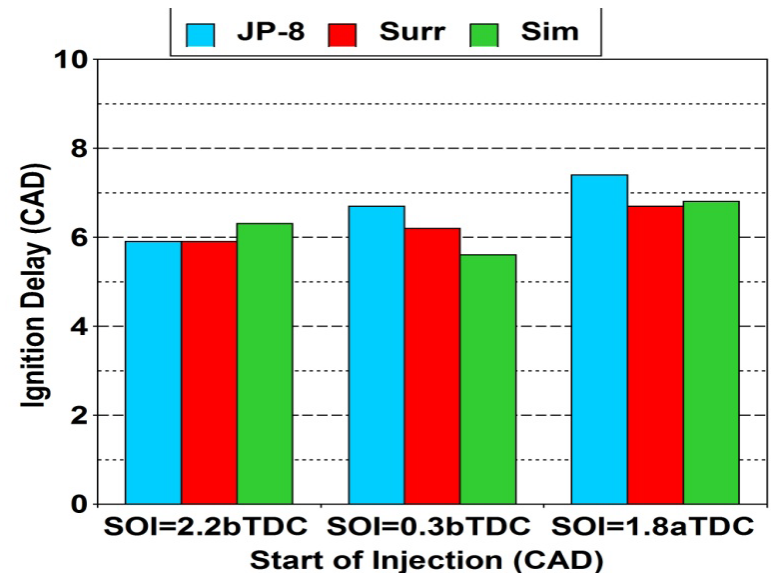


Figure 6. Comparison of Ignition Delays

Results: Experiments/3D CFD Simulation

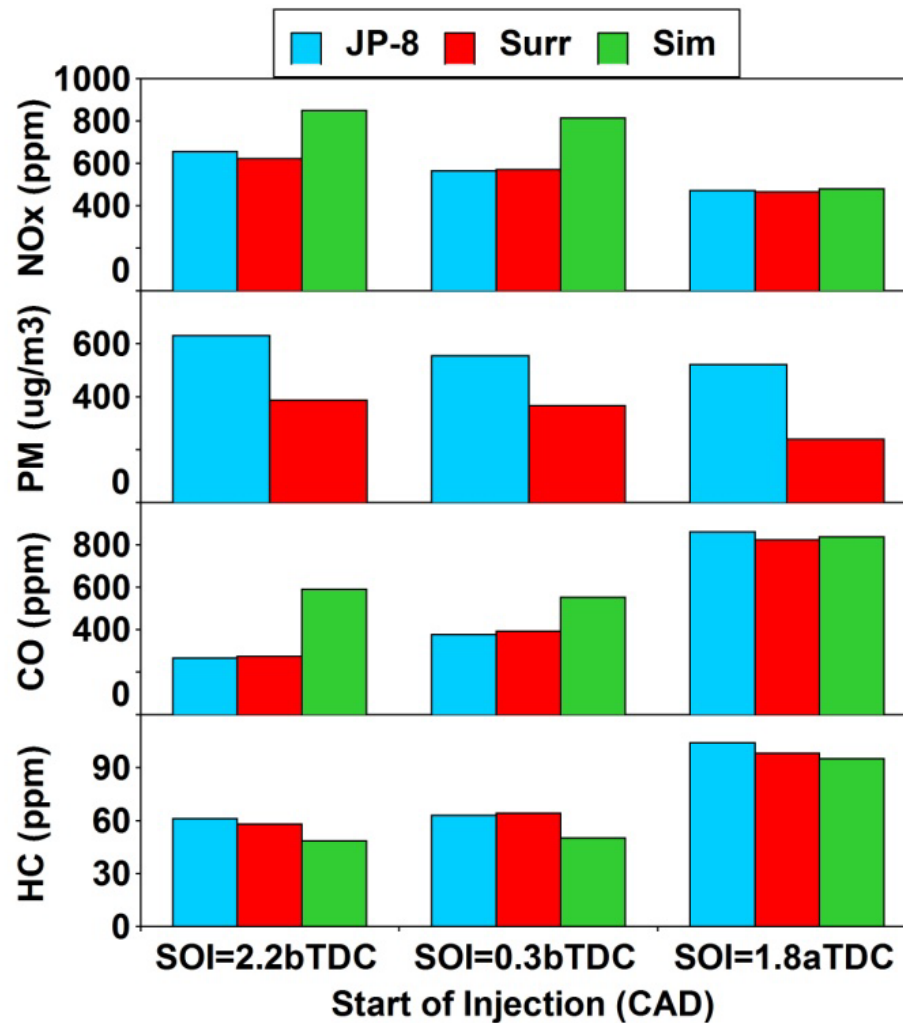


Figure 7. Comparisons of engine-out emissions

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Experimental Validation:

- At the test conditions analyzed, the two-component S2 surrogate fairly reproduced the following characteristics of the target JP-8:
 - Ignition delays
 - Pressure, RHR, mass-averaged gas temperature
 - Engine-out emissions (CO, HC, NOX), with an exception of the absolute PM values

3D CFD Simulation:

- The simulation results were in fairly good agreement with the experimental data for the surrogate

The two-component S2 surrogate could be a reasonable choice for its use in further investigations on the target JP-8

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Thank You